

Phase Transitions of Ferromagnetic Potts Models on the Simple Cubic Lattice

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We investigate the 2- and 3-state ferromagnetic Potts models on the simple cubic lattice using the tensor renormalization group method with higher-order singular value decomposition (HOTRG). HOTRG works in the thermodynamic limit, where we use the Z_q symmetry of the model, combined with a new measure for detecting the transition, to improve the accuracy of the critical point for the 2-state model by two orders of magnitude, obtaining $T_c = 4.51152469(1)$. The 3-state model is far more complex, and we improve the overall understanding of this case by calculating its thermodynamic quantities with high accuracy. Our results verify the first-order nature of the phase transition and the HOTRG transition temperature benchmarks the most recent Monte Carlo result.

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The phase transitions of the Potts model have for decades served as an important paradigm for the study of critical properties, not only in hard and soft condensed matter physics but also in fields as diverse as high-energy physics and biophysics [1, 2]. While the majority of these studies have been for systems in two spatial dimensions, the three-dimensional (3D) Potts model also contains independent and valuable insight for many problems. As examples, the three-state ($q = 3$) 3D ferromagnetic Potts model plays an important role in describing the finite-temperature deconfining phase transition and the structure of quantum chromodynamics (QCD) [3–5], while the antiferromagnetic Potts model with $q \geq 3$ can be used to study entropy-driven phase transitions in 3D [6–9].

The nature of the phase transition that occurs in the 3D three-state ferromagnetic Potts model was in the past the subject of extended controversy [10–13]. Most authors now favor a weakly first-order transition [5, 14–19], although a rigorous argument remains absent. In fact it is currently believed that the 3D q -state ferromagnetic Potts model possesses a first-order phase transition for all $q \geq 3$ and a continuous transition only when $q = 2$ (the Ising case) [19, 20]. The latent heat, which measures the strength of the first-order nature, grows with q [20].

The tensor renormalization group (TRG) method [21–24] is a type of coarse-graining real-space renormalization technique, and continues to draw increasing interest in condensed matter, statistical, and computational physics. One of its primary advantages is that it is intrinsically in the thermodynamic limit, yielding direct and highly accurate results with no need for finite-size scaling (as in density matrix renormalization group (DMRG) [25], Monte Carlo, and other numerical techniques). TRG-based methods have been studied systematically [22–24] and applied with considerable success to statistical spin models [26–29], gauge models [30, 31], and even quantum lattice models [32–35].

In this paper, we employ the recently developed TRG method based on higher-order singular value decompo-

sition (HOSVD), abbreviated as HOTRG [24], to study the thermodynamic properties of the 2- and 3-state ferromagnetic Potts models on the simple cubic lattice. The general ferromagnetic q -state Potts model [1], which may be considered as an extension of the Ising model to more than two components, is defined by the Hamiltonian

$$H = - \sum_{\langle ij \rangle} \delta_{s_i s_j}, \quad (1)$$

where the sum is over all nearest-neighbor lattice sites and $s_i = 0, 1, \dots, q-1$ denotes the q different Potts states on site i .

The partition function of any classical statistical model with only local interactions, a category to which the Potts model belongs, can always be represented by a tensor-network model [21, 23]. To construct this tensor network, we first expand the Boltzmann factor as

$$e^{\beta \delta_{s_i s_j}} = \sum_{t=0}^{q-1} Q_{s_i t} Q_{s_j t}^*,$$

where

$$Q_{s_i t} = e^{i 2 \pi t s_i / q} \sqrt{\frac{e^{\beta} - 1 + q \delta_{t,0}}{q}}, \quad (2)$$

and the superscript $(*)$ denotes complex conjugation. The local tensor may then be defined [23] as

$$T_{x_i x'_i y_i y'_i z_i z'_i} = \sum_{s_i} Q_{s_i x_i} Q_{s_i x'_i}^* Q_{s_i y_i} Q_{s_i y'_i}^* Q_{s_i z_i} Q_{s_i z'_i}^*, \quad (3)$$

where $(x_i, x'_i, y_i, y'_i, z_i, z'_i)$ are respectively the tensor indices for the x, y , and z directions, and is represented schematically in Fig. 1(a). The partition function is represented in terms of these tensors by

$$Z = \text{Tr} \prod_i T_{x_i x'_i y_i y'_i z_i z'_i}, \quad (4)$$

where the trace is over all repeated indices.

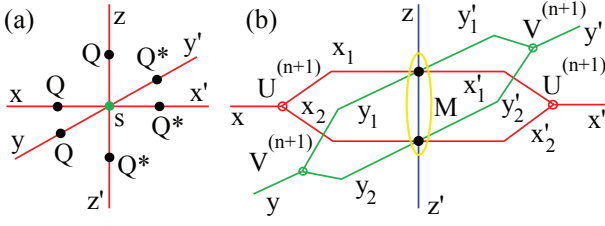


FIG. 1. (a) A local tensor is defined by summing over the common index s . (b) Renormalization step updating the local tensor by z -axis contraction.

In 2D, tensor-network models can be evaluated easily by using TRG methods that contract the network efficiently. However, the evaluation of 3D tensor networks was an intractable problem, in terms of computational effort and accuracy, until the proposal of HOTRG [24]. Specializing our description to the simple cubic lattice, we assume for simplicity that all local tensors T are identical. At the n th renormalization step of HOTRG, one first contracts two adjacent tensors with a common index i along the z -direction to form a new tensor M ,

$$M_{ijklzz'}^{(n)} = \sum_{\tilde{z}} T_{x_1 x'_1 y_1 y'_1 z \tilde{z}}^{(n)} T_{x_2 x'_2 y_2 y'_2 \tilde{z} z'}^{(n)}, \quad (5)$$

where $i = x_1 \otimes x_2$, $j = x'_1 \otimes x'_2$, $k = y_1 \otimes y_2$, and $l = y'_1 \otimes y'_2$. Clearly the bond dimension of the new tensor in the x and y directions is the square of that in the original tensor, and a truncation scheme is necessary to avoid an exponential divergence.

To perform an optimal truncation, HOTRG employs the HOSVD to decompose $M^{(n)}$ as

$$M_{ijklzz'}^{(n)} = \sum_{xx'yy'mn} S_{xx'yy'mn} U_{ix}^L U_{jx'}^R U_{ky}^F U_{ly'}^B U_{zm}^U U_{z'n}^D, \quad (6)$$

where the matrices U are all unitary and S is known as the core tensor, one with the properties of full orthogonality and pseudo-diagonality [36]. Details of the practical determination of the six unitary matrices may be found in Ref. [24]. Next one compares the values of

$$\varepsilon_1 = \sum_{i>D} |S_{i,::,::,::}| \text{ and } \varepsilon_2 = \sum_{i>D} |S_{:,i,::,::}|, \quad (7)$$

where D is the bond dimension retained after truncation.

$$|S_{i,::,::,::}| = \sqrt{\sum_{x'y'y'z'} S_{ix'y'y'z'}^2}$$

is the norm of the subtensor $S_{i,::,::,::}$ and $|S_{:,i,::,::}|$ is defined similarly. If $\varepsilon_1 < \varepsilon_2$ (or $\varepsilon_1 > \varepsilon_2$), one truncates the second dimension of U^L (or U^R) to D to form an isometry $U^{(n+1)}$. A similar treatment applied to the y -direction yields another isometry $V^{(n+1)}$, with which the renormalized local tensor is then updated as

$$T_{xx'yy'zz'}^{(n+1)} = \sum_{ijkl} M_{ijklzz'}^{(n)} U_{ix}^{(n+1)} U_{jx'}^{(n+1)} V_{ky}^{(n+1)} V_{ly'}^{(n+1)}. \quad (8)$$

The schematic representation of this process is shown in Fig. 1(b). This type of truncation scheme provides a good local approximation to minimize the truncation error and to conserve the optimal amount of information about the system. In practical calculations, the lattice is contracted along the x , y , and z directions in sequence until the desired quantities have converged.

Clearly the size of the lattice is reduced by a factor of 2 after an HOTRG step. Alternatively stated, n HOTRG steps represent a system of size 2^n , and with sufficiently large n it is easy to approach the thermodynamic limit. In practice $n = 30$ is enough for most systems. This sort of size is inordinately difficult to reach by other methods such as Monte Carlo, and it is this convenience with which HOTRG can access the infinite system, instead of requiring a finite-size scaling analysis, which is one of its prime advantages over other methods. In general, the accuracy of HOTRG is limited by the local truncation error and the bond dimension D retained during the renormalization step. In 3D, the computational complexity and the memory cost of the HOTRG algorithm scale respectively as D^{11} and D^6 [24].

One means of increasing the accessible bond dimension is to make full use of the symmetries of the Hamiltonian, an approach employed in all numerical methods to eliminate unnecessary memory use and redundant computation [23], thus reducing the computational cost quite significantly. The q -state Potts model possesses Z_q symmetry and it is straightforward to show that the elements of the initial local tensor $T_{x_i x'_i y_i y'_i z_i z'_i}$ (3) are nonzero only when the indices satisfy the relation

$$\text{mod}(x_i + y_i + z_i, q) = \text{mod}(x'_i + y'_i + z'_i, q). \quad (9)$$

One may further verify that this relation is maintained throughout the renormalization procedure, which is of vital importance in practical calculations.

We seek an accurate measure appropriate to the TRG scheme to fix the transition point explicitly. After sufficiently many renormalization steps, T approaches a fixed-point tensor which behaves differently in different phases. A quantitative measure for this difference, introduced in Ref. [37], is

$$X = \frac{(\text{Tr} A)^2}{\text{Tr}(A^2)}, \quad (10)$$

where A is a $D \times D$ matrix defined by

$$A_{z_i z'_i} = \sum_{x_i y_i} T_{x_i x_i y_i y_i z_i z'_i}. \quad (11)$$

For the fixed point tensor T in the high-temperature disordered phase, all eigenvalues of A are close to zero other than the first, whereas in the low-temperature symmetry-breaking phase the first q eigenvalues are approximately equal with the others zero. Thus the degeneracy of the

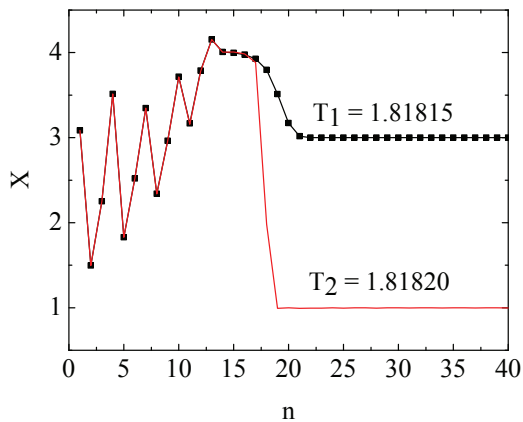


FIG. 2. Evolution of X with the number n of RG steps in HOTRG calculations for the $q = 3$ Potts model with $D = 16$. Values are shown for two temperatures $T_1 = 1.81815$ and $T_2 = 1.81820$, which are in the ordered and disordered phases respectively. Although T_1 and T_2 are very close, X approaches one of two explicitly different values, q or 1 , when $n > 20$, indicating clearly that a phase transition occurs at $T_1 < T < T_2$.

largest eigenvalue of A can be used as an indicator of symmetry-breaking, and is given by the value of X . Figure 2 shows the behavior of X for the $q = 3$ Potts model during the renormalization group (RG) flow at two temperatures differing by only 5×10^{-5} . The almost exact convergence of X to the values q or 1 beyond $n = 20$ illustrates the power of this approach.

The HOTRG method was first applied to study the 3D Ising model (the $q = 2$ Potts model on the simple cubic lattice) in Ref. [24]. There the maximum attainable bond dimension was $D = 16$, with which the accuracy of the critical temperature T_c was comparable to the best Monte Carlo result. In this work, by employing the Z_q symmetry, we increase D to 23. As shown in Fig. 3, the critical temperature T_c converges very accurately beyond $D = 13$, to the value $T_c = 4.51152469(1)$. Table I shows

TABLE I. Comparison of critical temperatures T_c obtained by different methods for the Ising model on the simple cubic lattice.

Method	T_c
CTMRG (2001) [38]	4.5393
TPVA (2005) [39]	4.554
Algebraic variation (2006) [40]	4.547
Series expansion (2000) [41]	4.511536(21)
Monte Carlo RG (1996) [42]	4.5115(2)
Monte Carlo (2003) [43]	4.5115248(6)
Monte Carlo (2010) [44]	4.5115232(17)
HOTRG ($D = 16$) (2012) [24]	4.511544
HOTRG ($D = 23$, this work)	4.51152469(1)

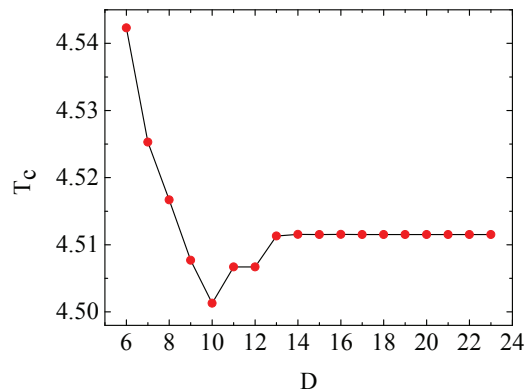


FIG. 3. Critical temperature T_c as a function of the bond dimension D obtained by HOTRG for the Ising model on the simple cubic lattice.

the comparison with results obtained for T_c in this model by other methods. To our knowledge, our result is two orders of magnitude more precise than the best alternative treatment to date (Monte Carlo) and six orders more precise than the results obtained by the corner transfer matrix renormalization group (CTMRG) and the tensor product variational approach (TPVA) introduced by Nishino and coworkers [19, 38, 39]. This result displays both the power of the Z_q symmetry and the accuracy of the HOTRG algorithm at higher D , even compared to other tensor-based approaches.

We now turn to the 3-state Potts model, which is significantly more challenging and less well understood. We first illustrate the thermodynamic quantities computed by HOTRG, for which $D = 14$ provides representative results (as shown below). We have calculated the internal energy E , the specific heat C , and the ferromagnetic magnetization $M = \sum_i \delta_{s_i,0}/N$. In Fig. 4(b) one observes a sharp peak in the specific-heat curve, indicative of a phase transition. That this transition has first-order nature is demonstrated by the corresponding discontinuity in the energy curve around $T = 1.819$, shown in Fig. 4(a). With a temperature resolution of 10^{-5} [inset, Fig. 4(a)], the latent heat ΔE , which denotes the energy difference between the two phases at the critical point, is clearly finite, with a value $\Delta E = 0.2029$ for $D = 14$. A comparison of the results obtained for this quantity by different methods is shown in Table II; while the HOTRG result is fully consistent with the spread of available values, we make no claims concerning the quantitative accuracy of the $D = 14$ value, and compute it primarily to confirm the qualitative nature of the transition.

Figure 4(c) shows the behavior of the magnetization, which decreases smoothly from 1 until T approaches the critical point, where it falls sharply to a value of $1/3$. When $T = 0$, the ferromagnetic interaction aligns all the spins and $M = 1$. As T grows, increasing thermal fluctuations cause the steady decrease, but the system re-

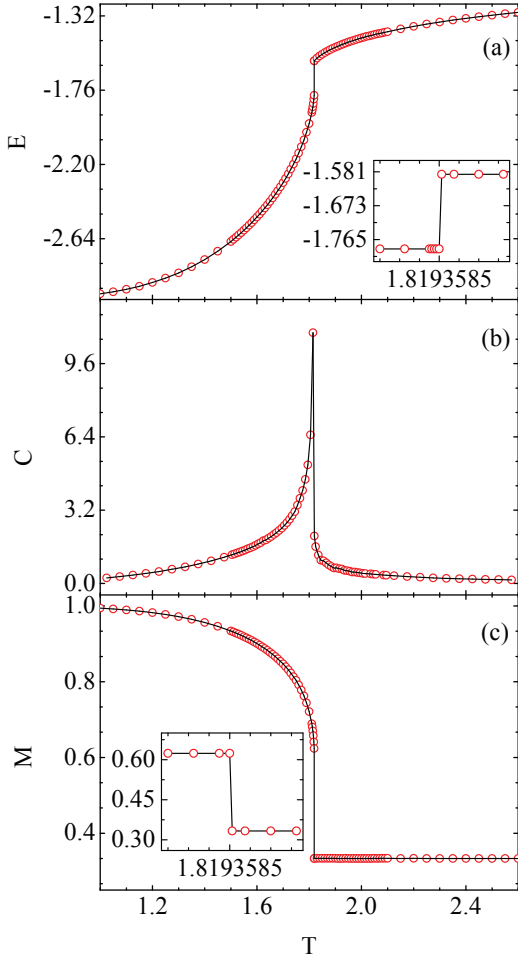


FIG. 4. (a) Internal energy per site, (b) specific heat, and (c) magnetization computed as functions of temperature by HOTRG for the $q = 3$ ferromagnetic Potts model on the simple cubic lattice with bond dimension $D = 14$. Insets in panels (a) and (c) show respectively the discontinuities in internal energy and magnetization at the phase transition which indicate its first-order nature.

mains in the symmetry-broken phase. Only when $T > T_c$ does the system enter the fully disordered phase, where $M = 1/3$ (all spin components equal). Once again the first-order nature of the transition is clearly visible in the sharp drop of the order parameter at T_c [inset, Fig. 4(c)], which is $\Delta M = 0.2903$ for $D = 14$.

A more accurate estimate of T_c is essential for the study of critical properties, and for this we exploit the symmetry of the tensor-network model to raise the bond dimension to $D = 21$. From the temperature dependence of X we obtain $T_c = 1.8165945$ for $D = 21$ [inset, Fig. 5]. However, because the accuracy of HOTRG improves at larger bond dimensions (Fig. 3), it is necessary to investigate the behavior of T_c with D . We show in Fig. 5 the convergence of T_c for the $q = 3$ case, where it is clear that the results are not yet in the convergent regime for any accessible D values. However, because they have al-

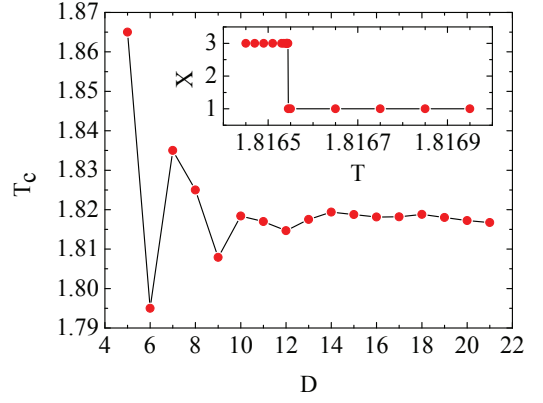


FIG. 5. Transition temperature T_c as a function of bond dimension D for the $q = 3$ ferromagnetic Potts model on the simple cubic lattice. Inset: behavior of X (Eq.10) as a function of temperature for $D = 21$, where the abrupt step in the curve gives a phase transition at $T_c = 1.8165945$.

most converged for $D = 21$, we are currently able to estimate the true transition temperature and error bar as $T_c = 1.8166(5)$, which sets a valuable additional benchmark. A comparison of T_c obtained by different methods is shown in Table II, where the $D = 21$ HOTRG result agrees well (relative error 10^{-4}) with the most recent Monte Carlo simulations [5].

On the other hand, the lack of convergence even by the most sophisticated HOTRG methods and measures indicates that the 3-state Potts model is a genuinely hard problem. To achieve the same type of convergence as in the Ising model, within the same calculational framework, requires a still larger tensor dimension D , which is

TABLE II. Comparison of latent heats ΔE and transition temperatures T_c for the $q = 3$ ferromagnetic Potts model on the simple cubic lattice obtained by different methods. The tensor bond dimensions retained in the HOTRG calculations of ΔE and T_c were respectively $D = 14$ and $D = 21$. L denotes the largest system size (cube side) reached in the Monte Carlo simulations.

Method	ΔE	T_c
Series expansion (1979) [48]		1.7289(12)
Monte Carlo RG (1979) [14]		1.818
Monte Carlo (1982, $L = 8$) [45]	0.12	1.81
Pair approximation (1982) [45]	0.123	1.879
Monte Carlo (1987, $L = 16$) [46]	0.2222(7)	1.81618(7)
Monte Carlo (1991, $L = 36$) [47]	0.16062(52)	1.816455(35)
Monte Carlo (1997, $L = 36$) [18]	0.1614(3)	1.816316(33)
Monte Carlo (2007, $L = 50$) [5]	0.1643(8)	1.816315(19)
TPVA (2002) [19]	0.228	1.8195
HOTRG (this work)	0.2029	1.8166
	($D = 14$)	($D = 21$)

computationally intensive in both time and memory. An alternative approach is to include the effect of the bond environment for a global optimization of the truncation during the coarse-graining process, as in the highly efficient second renormalization group method [22, 24]. By comparison with previous work for both the $q = 2$ and 3 Potts models, it is clear that the HOTRG method already offers comparable results for the challenging $q = 3$ case (Table II) and that it has very significant potential for improvement, as already achieved for the $q = 2$ case (Table I).

In summary, we have investigated the 2- and 3-state ferromagnetic Potts models on the simple cubic lattice by using the recently developed tensor renormalization group technique, which can study the thermodynamic limit directly with no need for finite-size scaling. By employing the refined HOTRG method, exploiting the Z_q symmetry of the Hamiltonians, and introducing a TRG-specific measure for the ground-state properties, we have determined the phase-transition temperature to high accuracy. For the 2-state model with $D = 23$, we have obtained, to our knowledge, by far the most accurate critical temperature of any available method, $T_c = 4.51152469(1)$. For the 3-state model with $D = 14$, we have calculated the thermodynamic quantities with high precision, specifically the internal energy, latent heat, specific heat, and magnetization. These results verify the first order nature of the symmetry-breaking phase transition. By reaching $D = 21$ we obtain a phase-transition temperature $T_c = 1.8166$, which is close to the extrapolated Monte Carlo result.

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[1] R. B. Potts, Proc. Cambridge Philos. Soc. **48**, 106 (1952).
 [2] F. Y. Wu, Rev. Mod. Phys. **54**, 235 (1982).
 [3] B. Svetitsky and L. G. Yaffe, Nucl. Phys. B **210**, 423 (1982).
 [4] B. A. Berg, H. Meyer-Ortmanns, and A. Velytsky, Phys. Rev. D **70**, 054505 (2004).
 [5] A. Bazavov and B. A. Berg, Phys. Rev. D **75**, 094506 (2007).
 [6] J. R. Banavar, G. S. Grest, and D. Jasnow, Phys. Rev. Lett. **45**, 1424 (1980); Phys. Rev. B **25**, 4639 (1982).
 [7] Y. Ueno, G. Sun, and I. Ono, J. Phys. Soc. Jpn. **58**, 1162 (1989).
 [8] S. Wang, R. H. Swendsen, and R. Kotecky, Phys. Rev. Lett. **63**, 109 (1989); Phys. Rev. B **42**, 2465 (1990).
 [9] A. Rosengren and S. Lapinskas, Phys. Rev. Lett. **71**, 165 (1993).
 [10] R. V. Ditzian and J. Oitmaa, J. Phys. A **7**, 16 (1974).

[11] J. P. Straley, J. Phys. A **7**, 2173 (1974).
 [12] I. G. Enting, J. Phys. A **7**, 1617 (1974).
 [13] H. J. Herrmann, Z. Phys. B **35**, 171 (1979).
 [14] H. W. J. Blote and R. H. Swendsen, Phys. Rev. Lett. **43**, 799 (1979).
 [15] S. J. K. Jensen and O. G. Mouritsen, Phys. Rev. Lett. **43**, 1736 (1979).
 [16] M. Fukugita and M. Okawa, Phys. Rev. Lett. **63**, 13 (1989).
 [17] J. Lee and J. M. Kosterlitz, Phys. Rev. B **43**, 1268 (1991).
 [18] W. Janke and R. Villanova, Nucl. Phys. B **489**, 679 (1997).
 [19] T. Nishino, K. Okunishi, Y. Hieida, N. Maeshima, and Y. Akutsu, Nucl. Phys. B **575**, 504 (2000); A. Gendiar and T. Nishino, Phys. Rev. E **65**, 046702 (2002).
 [20] A. Bazavov, B. A. Berg, and S. Dubey, Nucl. Phys. B **802**, 421 (2008).
 [21] M. Levin and C. P. Nave, Phys. Rev. Lett. **99**, 120601 (2007).
 [22] Z. Y. Xie, H. C. Jiang, Q. N. Chen, Z. Y. Weng, and T. Xiang, Phys. Rev. Lett. **103**, 160601 (2009).
 [23] H. H. Zhao, Z. Y. Xie, Q. N. Chen, Z. C. Wei, J. W. Cai, and T. Xiang, Phys. Rev. B **81**, 174411 (2010).
 [24] Z. Y. Xie, J. Chen, M. P. Qin, J. W. Zhu, L. P. Yang, and T. Xiang, Phys. Rev. B **86**, 045139 (2012).
 [25] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
 [26] Q. N. Chen, M. P. Qin, J. Chen, Z. C. Wei, H. H. Zhao, B. Normand, and T. Xiang, Phys. Rev. Lett. **107**, 165701 (2011).
 [27] Y. Meurice, Phys. Rev. B **87**, 064422 (2013).
 [28] E. Efrati, Z. Wang, A. Kolan, and L. P. Kadanoff, unpublished (arXiv:1301.6323).
 [29] J. F. Yu, Z. Y. Xie, Y. Meurice, Y. Liu, A. Denbleyker, H. Zou, M. P. Qin, J. Chen, and T. Xiang, Phys. Rev. E **89**, 013308 (2014).
 [30] Y. Liu, Y. Meurice, M. P. Qin, J. U. Yockey, T. Xiang, Z. Y. Xie, J. F. Yu, and H. Zou, Phys. Rev. D **88**, 056005 (2013).
 [31] A. Denbleyker, Y. Liu, Y. Meurice, M. P. Qin, T. Xiang, Z. Y. Xie, J. F. Yu, and H. Zou, Phys. Rev. D **89**, 016008 (2014).
 [32] H. C. Jiang, Z. Y. Weng, and T. Xiang, Phys. Rev. Lett. **101**, 090603 (2008).
 [33] Z. C. Gu, M. Levin, and X. G. Wen, Phys. Rev. B **78**, 205116 (2008).
 [34] H. H. Zhao, C. Xu, Q. N. Chen, Z. C. Wei, M. P. Qin, G. M. Zhang, and T. Xiang, Phys. Rev. B **85**, 134416 (2012).
 [35] Z. Y. Xie, J. Chen, J. F. Yu, X. Kong, B. Normand, and T. Xiang, Phys. Rev. X **4**, 011025 (2014).
 [36] L. de Lathauwer, B. de Moor, and J. Vandewalle, SIAM J. Matrix Anal. Appl. **21**, 1253 (2000).
 [37] Z. C. Gu and X. G. Wen, Phys. Rev. B **80**, 155131 (2009).
 [38] T. Nishino, Y. Hieida, K. Okunishi, N. Maeshima, Y. Akutsu, and A. Gendiar, Prog. Theo. Phys. **105**, 409 (2001).
 [39] A. Gendiar and T. Nishino, Phys. Rev. B **71**, 024404 (2005).
 [40] S. G. Chung, Phys. Lett. A **359**, 707 (2006).
 [41] P. Butera and M. Comi, Phys. Rev. B **62**, 14837 (2000).
 [42] R. Gupta and P. Tamayo, Int. J. Mod. Phys. C **7**, 305 (1996).
 [43] Y. J. Deng and H. W. J. Blote, Phys. Rev. E **68**, 036125 (2003).

- [44] M. Hasenbusch, Phys. Rev. B **82**, 174433 (2010).
- [45] I. Ono and K. Ito, J. Phys. C **15**, 4417 (1982).
- [46] W. G. Wilson and C. A. Vanse, Phys. Rev. B **36**, 587 (1987).
- [47] N. A. Alves, B. A. Berg, and R. Villanova, Phys. Rev. B **43**, 5846 (1991).
- [48] S. Miyashita, D. D. Betts, and C. J. Elliott, J. Phys. A **12**, 1605 (1979).